Renormalization for reaction-front propagation in a fully developed turbulent shear flow

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A crude upper bound for the ensemble averaged speed of a reaction front in a fully developed turbulent shear flow has been derived from the Kolmogorov-Petrovskii-Piskunov equation modified by the convection term with Gaussian velocity field exhibiting long range correlations and infrared divergence in the limit of large Reynolds number. The analysis involves a singular perturbation for small values of the ratio of the Kolmogorov length scale to the integral length scale of turbulent flow; the principal tools used are a functional integral technique and a renormalization procedure. The basic physical result is that the infrared divergence of a random velocity field may lead to the acceleration of a coarse-grained reaction front.

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I. INTRODUCTION

In recent years reaction-front propagation in a turbulent flow has been studied in the physics literature [1–6] due to its great practical significance as a model for premixed turbulent combustion in the so-called flamelet regime [7–10]. Most of these studies have been directed towards determination of the macroscale propagation rate of a front and its parametric dependence on the statistical characteristics of random velocity fields. Although significant progress has already been made in the solution of this problem, especially by using the G equation describing the front propagation by the Huygens mechanism [1, 7–10], still there exist many open problems including how to derive the formula for the propagation rate in the long-time, large-distance limit from *the first principle.*

In this paper we choose as a convenient *starting point* the Kolmogorov-Petrovskii-Piskunov (KPP) equation [11] modified by the convection term with a homogeneous random velocity field. In general this is an extremely complex problem, therefore it seems to be reasonable to set up a simple but nontrivial model for turbulent velocity field. The first steps in this direction were made by Souganidis and Majda [12] (see also [13]) who studied large scale reaction-front dynamics with KPP chemistry and turbulent convection involving two separated length scales for the random velocity field. They derived renormalized effective equations for large scale reaction-front propagation and what is more showed that the renormalized evolution of reaction front is governed by a variational inequality rather than a simple Huygens principle.

Here we adopt the model of turbulent shear flow with *arbitrary many spatial scales* introduced in [14,15]. Our primary interest is to describe the reaction front propagation on length and time scales that are larger than the integral length scale of turbulence and corresponding turnover time scale and derive a crude upper bound for the ensemble-averaged reaction-front position and speed.

II. KPP EQUATION WITH RANDOM CONVECTION TERM

We consider the following nondimensional Kolmogorov-Petrovskii-Piskunov (KPP) equation for a scalar field $\varphi(t,x,y)$

$$\frac{\partial\varphi}{\partial t}+v(t,x)\frac{\partial\varphi}{\partial y}=D\left(\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{\partial y^2}\right)+c(\varphi)\,\varphi\,, \qquad (1)$$

where the nonlinear source term $c(\varphi)\,\varphi$ is of KPP type, i.e.,

$$c\equiv c(0)=\max_{\varphi\in[0,1]} c(\varphi)\,>0\,, \qquad c(1)=0\,. \qquad (2)$$

Equation (1) incorporates the combined effects of random advection, diffusion, and nonlinearity. It has been made dimensionless by the Kolmogorov length scale $\eta=(\nu^3/\bar{\varepsilon})^{1/4}$, velocity scale $v_k=(\nu\bar{\varepsilon})^{1/4}$, and time scale $t_k=\nu/v_k$. Here $\bar{\varepsilon}$ is the average rate of dissipation of turbulent energy and ν is the viscosity which is also used to nondimensionalize the diffusion coefficient.

The random velocity $v(t,x)$ is assumed to be a homogeneous Gaussian field with a zero mean and a correlation function given by [14,15]

$$\langle v(t,x)\,v(t',x')\rangle=V^2\int\exp\{ik(x-x')-a|k|^z|t-t'|\}\times\psi_0\left(\frac{|k|}{\epsilon}\right)\,\psi_\infty(|k|)|k|^{-\sigma}\,dk\,, \qquad (3)$$

where $\psi_0(z)$ and $\psi_\infty(z)$ represent infrared and ultraviolet

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cutoffs correspondingly and satisfy

$$\psi_0(z) = \begin{cases} 0 & \text{if } |z| < z_0 \\ 1 & \text{if } |z| > z_1 \,, \end{cases}$$
$$\psi_\infty(z) = \begin{cases} 1 & \text{if } |z| < z_3 \\ 0 & \text{if } |z| > z_4. \end{cases} \tag{4}$$

The correlation function (3) involves three important nondimensional parameters σ, z, and ϵ. The dynamic exponent z describes the scaling of k-dependent "turnover" time $\tau(k) = 1/a \mid k \mid^z$ with the wave number k. The parameter σ is a natural characteristic of the spartial correlations of the velocity field. Both z and σ will play a very important role in what follows (for further discussion on these exponents see [14,15]). The small parameter ϵ is the ratio between the Kolmogorov length scale η and the integral length scale l_0, that is, $\epsilon = \mathrm{Re}^{-3/4}$, where $Re = u_0 l_0/\nu$ is the Reynolds number.

In this paper we choose to specify only the simplest form of the initial condition, namely

$$\varphi(0,x,y) = \chi(y) = \begin{cases} 1, & y \le 0 \\ 0, & y > 0 \,. \end{cases} \tag{5}$$

More general choice of the initial scalar field φ can also be made. In this case, new phenomena such as a spontaneous front propagation may occur [16].

III. TRAVELING WAVES AND UPPER BOUND ON ENSEMBLE-AVERAGED REACTION FRONT SPEED

It is well known [11] that if there is no convection term in (1) then there exists a traveling wave solution to (1)–(5),

$$\psi(t - uy) \qquad \text{as} \qquad t \to \infty \,, \tag{6}$$

where $\psi(z)$ is a monotonically decreasing function such that $\psi(-\infty) = 1\,, \psi(\infty) = 0$, and $u = \sqrt{4Dc}$ is the wave speed. Moreover, one can show that after a rescaling $t \to t/\epsilon$, $y \to y/\epsilon$ the wave profile (6) tends to a unit step function $\chi(t - uy)$ as $\epsilon \to 0$.

The question naturally arises as to whether the full nonlinear problem (1)–(5) has a traveling wave solution in the long-time, large-distance limit, and if so, what is the rate at which this coarse-grained wave propagates throughout a turbulent flow. It is tempting to suppose that there exists a scaling function $\lambda(\epsilon)$ such that $\lim_{\epsilon\to 0} \lambda(\epsilon) = 0$ for which the ensemble average of the solution of (1)–(5)

$$\left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle \qquad \text{as } \epsilon \to 0, \tag{7}$$

can be viewed as a wave propagating with a certain speed.

In this paper we shall analyze the asymptotic behavior of (7) by assuming that in the limit $\epsilon \to 0$ the ensemble average (7) develops a reaction front dividing the space in two regions, so that

$$\lim_{\epsilon\to 0} \left\langle \varphi\left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle = \begin{cases} 1, & G(t,y) > 0, \ -\infty < x < \infty \\ 0, & G(t,y) < 0, \ -\infty < x < \infty. \end{cases} \tag{8}$$

It is clear from (8) that the equation $G(t,y) = 0$ determines the position of the front. In this paper we propose the following formula for $G(t,y)$:

$$G(t,y) = \lim_{\epsilon\to 0} \lambda(\epsilon) \ln \left\langle \varphi^*\left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle \,, \tag{9}$$

where φ^* is a solution of (1)–(5) for the case in which the nonlinear function $c(\varphi)$ is replaced by its maximum value c.

The scaling function $\lambda(\epsilon)$ must be determined from the requirement that the limit (9) is nontrivial. To solve this problem we will follow the exact renormalization theory for eddy diffusivity developed in [14,15]. The function $\lambda(\epsilon)$ clearly depends on the specific choice of the exponents σ and z in the correlation function (3). In this paper we consider those values of the spectral parameters σ and z for which the energy of velocity is divergent in the limit of high Reynolds number, i.e., $\langle v^2\rangle \to \infty$ as $\epsilon \to 0$. One can expect that this infrared divergence gives rise to a nontrivial scaling behavior.

Now we wish to find an explicit expression for $G(t,y)$. The procedure is similar to that of Freidlin [16] (see also [17–20]) who has given a rigorous basis for the consideration of the nonlinear equations of KPP type in terms of a functional integral technique.

Applying the scaling transformation

$$t \to \frac{t}{\lambda(\epsilon)}, \qquad x \to \frac{x}{\epsilon}, \qquad y \to \frac{y}{\epsilon} \tag{10}$$

we can get an equation for $\varphi^\epsilon(t,x,y) = \varphi(\frac{t}{\lambda}, \frac{x}{\epsilon}, \frac{y}{\epsilon})$,

$$\frac{\partial \varphi^\epsilon}{\partial t} + \frac{\epsilon}{\lambda} v\left(\frac{t}{\lambda}, \frac{x}{\epsilon}\right)\frac{\partial \varphi^\epsilon}{\partial y} = \frac{\epsilon^2 D}{\lambda}\left(\frac{\partial^2 \varphi^\epsilon}{\partial x^2} + \frac{\partial^2 \varphi^\epsilon}{\partial y^2}\right) + \frac{1}{\lambda} c(\varphi^\epsilon)\,\varphi^\epsilon \,,$$

$$\varphi^\epsilon(0,x,y) = \chi(y) \,. \tag{11}$$

The initial-value problem (11) can be turned into the functional integral equation [16]

$$\varphi^\epsilon(t,x,y) = \mathbf{E}\,\chi(y(t)) \exp\left\{ \frac{1}{\lambda}\int_0^t c(\,\varphi^\epsilon(t-s, x(s), y(s))\,)\, ds \right\}, \tag{12}$$

where $\mathbf{E}$ denotes the expectation over the trajectories $x(s)$ and $y(s)$ that are the solution of the following stochastic differential equations:

$$dx(s) = \left(\frac{2\epsilon^2 D}{\lambda}\right)^{1/2} dw_x(s)\,, \qquad x(0) = x\,,$$

$$dy(s) = \frac{\epsilon}{\lambda} v\Big(\frac{t-s}{\lambda}, \frac{x(s)}{\epsilon}\Big)\, ds + \left(\frac{2\epsilon^2 D}{\lambda}\right)^{1/2} dw_y(s)\,, \qquad y(0) = y\,. \tag{13}$$

Here $w_x(s)$ and $w_y(s)$ are the independent Wiener processes.

The major advantage of the formulation of the basic problem (1)–(5) or (11) in terms of the functional integral equation (12) is that it allows us to obtain relatively easily an upper bound for the ensemble average of φ^ϵ and thereby an upper bound for the ensemble-average speed of reaction front. By definition,

$$\langle\, \varphi^\epsilon(t,x,y)\,\rangle = \int \varphi^\epsilon(t,x,y)\, P[v]\, \mathcal{D}v\,, \tag{14}$$

where $P[v]$ is the probability density functional of the random velocity field $v(t,x)$. Since $e^{c(\varphi)} \leq e^c$, it follows from (12) and (14) that

$$\langle\, \varphi^\epsilon(t,x,y)\,\rangle \leq \left\langle\, \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle,$$

where

$$\left\langle \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle = \int \mathbf{E}\,\chi(\,y(t)\,)\, \exp\left(\frac{ct}{\lambda}\right) P[v]\, \mathcal{D}v\,. \tag{15}$$

By using the stochastic differential equations (13), we can rewrite (15) as

$$\begin{aligned}\left\langle \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle &= \int \mathbf{E}\chi\left[y + \frac{\epsilon}{\lambda}\int_0^t v\left(\frac{t-s}{\lambda}, \frac{x}{\epsilon} + \left(\frac{2D}{\lambda}\right)^{1/2} w_x(s)\right) ds + \left(\frac{2\epsilon^2 D}{\lambda}\right)^{1/2} w_y(t)\right] \\ &\quad \times \exp\left(\frac{ct}{\lambda}\right) P[v]\,\mathcal{D}v \\ &= \int \mathbf{E}\chi\left(y + \eta + \left(\frac{2\epsilon^2 D}{\lambda}\right)^{1/2} w_y(t)\right) \exp\left(\frac{ct}{\lambda}\right) p_\epsilon(\eta)\, d\eta\,,\end{aligned} \tag{16}$$

where

$$\eta = \frac{\epsilon}{\lambda}\int_0^t v\left(\frac{t-s}{\lambda}, \frac{x}{\epsilon} + \left(\frac{2D}{\lambda}\right)^{1/2} w_x(s)\right) ds \tag{17}$$

is a Gaussian variable and therefore the probability density function for it may be written as follows

$$p_\epsilon(\eta) = \frac{1}{\sqrt{4\pi S^w_\epsilon(t)\, t\, \lambda(\epsilon)}} \exp\left\{-\frac{\eta^2}{4R^w_\epsilon(t)\, t\, \lambda(\epsilon)}\right\}, \tag{18}$$

where

$$R^w_\epsilon(t) = \frac{\epsilon^2}{2t\,\lambda^3}\int_0^t\int_0^t \left\langle v\left(\frac{s-s'}{\lambda}, \left(\frac{2D}{\lambda}\right)^{1/2} [w_x(s) - w_x(s')]\right) v(0,0)\right\rangle ds ds'\,. \tag{19}$$

Since we are primarily concerned here with the effects of infrared divergence, in what follows we consider only the case in which the transport process is dominated by the random velocity field $v(t,x)$ and therefore the influence of the Brownian motion $w_x(t)$ and $w_y(t)$ may be neglected. In this case we have

$$\left\langle \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon}\right)\right\rangle = \int \chi(y+\eta)\, \frac{1}{\sqrt{4\pi R_\epsilon(t)\, t\, \lambda(\epsilon)}} \exp\left\{\frac{ct}{\lambda(\epsilon)} - \frac{\eta^2}{4R_\epsilon(t)\, t\, \lambda(\epsilon)}\right\} d\eta\,, \tag{20}$$

where

$$R_\epsilon(t) = \frac{\epsilon^2 V^2}{2t\lambda^3} \int_0^t \int_0^t \int \exp\Big\{ -\frac{a \mid k \mid^z}{\lambda} \mid s - s' \mid \Big\} \psi_0 \left(\frac{\mid k \mid}{\epsilon} \right) \psi_\infty(\mid k \mid) \mid k \mid^{-\sigma} dk ds ds' . \tag{21}$$

In the limit $\epsilon \to 0$ it is natural to seek an approximate expression of the form

$$\left\langle \varphi^* \left(\frac{t}{\lambda(\epsilon)}, \frac{x}{\epsilon}, \frac{y}{\epsilon} \right) \right\rangle \propto \exp\Big\{ \frac{G(t,y)}{\lambda(\epsilon)} \Big\}, \tag{22}$$

which allows us to find $G(t,y)$ and thereby the crude upper bound for the ensemble-average position of the reaction front without directly solving the nonlinear problem (1)–(5). It follows from (20)–(22) that

$$G(t,y) = \lim_{\epsilon \to 0} \lambda(\epsilon) \ln \left\langle \varphi \left(\frac{t}{\lambda(\epsilon)}, \frac{y}{\epsilon} \right) \right\rangle = ct - \frac{y^2}{4R_0(t)\,t}, \tag{23}$$

where

$$R_0(t) = \lim_{\epsilon \to 0} R_\epsilon(t) . \tag{24}$$

Our strategy now is to find $\lambda(\epsilon)$ such that the limit (24) is nontrivial. There exists a wide range of values of spectral parameters σ and z for which simple diffusive scaling $\lambda(\epsilon) = \epsilon$ leads to the infrared divergence of the integral (21) in the limit $\epsilon \to 0$. Therefore the renormalization procedure is needed to render $R_0(t)$ finite. The corresponding analysis of such a renormalization will not be repeated here since it follows closely that described in [14,15]. The final result may be written as follows:

$$R_0(t) = \begin{cases} R^A = \frac{V^2}{a} \int \psi_0(\mid k \mid) \mid k \mid^{-\sigma - z} dk & (A) \\ R^B = \frac{V^2 t}{2} \int \psi_0(\mid k \mid) \mid k \mid^{-\sigma} dk & (B) \\ R^C = V^2 a^{(\sigma-1)/z} \int \mid k \mid^{-\sigma-z} [1 - \mid k \mid^{-z} t^{-1} (1 - e^{-|k|^z t})]\, dk & (C) \end{cases} \tag{25}$$

with the anomalous scaling for three different regions (A), (B), and (C),

$$\lambda(\epsilon) = \begin{cases} \epsilon^{\frac{3-\sigma-z}{2}}, & 1 - z < \sigma < 3 - 3z\ ,\ 0 < z < 1 \quad (A) \\ \epsilon^{\frac{3-\sigma}{3}}, & 3 - 3z < \sigma < 3\ ,\ 0 < z < 2/3\ ;\ 1 < \sigma < 3\ ,\ z > 2/3 \quad (B) \\ \epsilon^{\frac{2z}{3z+\sigma-1}}, & 3 - 3z < \sigma < 1,\ 2/3 < z < 2 . \quad (C). \end{cases} \tag{26}$$

It is easy to check that the Brownian motion describing the molecular diffusion is negligible for the regions $(A) - (C)$. In the case of Kolmogorov statistics, we have $\sigma = 5/3$ and $z = 2/3$. These values correspond to the point lying in the region (B). It is interesting to note that in the renormalization theory for turbulent diffusion [14,15] the Kolmogorov spectrum corresponds to a boundary between two different scaling regions.

By equating $G(t,y)$ to zero, we find the upper bound for the ensemble-average position $y(t)$ and the propagation rate $u(t)$ of the reaction front in the long-time, large-distance limit

$$y(t) = (4cR_0(t))^{1/2}\, t, \quad u(t) = \frac{d}{dt}(4cR_0(t))^{1/2}\, t . \tag{27}$$

IV. DISCUSSION

The model of turbulent shear flow (3) and (4) appears to be very useful because the problem of ensemble-averaged reaction-front propagation for KPP equation can be solved in such an explicit fashion. Now we can see how the infrared divergence of random velocity field may lead not only to new scaling behavior, but what is more to the acceleration of the reaction front. It is clear from (25)–(27) that the upper bound for the propagation rate $u(t)$ increases with time for the regions (B) and (C). In particular, for the Kolmogorov turbulent shear flow the upper bound may be written as

$$u(t) = 3V \left(\frac{ct}{2} \int \psi_0(\mid k \mid) \mid k \mid^{-5/3} dk \right)^{1/2} .$$

The phenomenon of acceleration is physically due to the enhanced time-dependent effective turbulent diffusion in the y-direction. It is interesting to note that the same time dependence of the effective flame speed is observed for the spherical flames in the regime of well developed hydrodynamic instability [21].

In this paper attention has been focused only on the determination of the upper bound for the ensemble-averaged position and propagating rate of reaction front for the homogeneous case. New phenomena such as jumps of the reaction front, dependence of propagation speed on initial conditions, etc. [16], may occur when a nonlinear term is chosen to depend on the space coordinate after rescaling or in the case of velocity field varying on the integral length scale and non-homogeneous initial conditions. These problems can also be treated by the proposed method and we consider them in [22]. It should be noted that the preliminary work done here might be of big practical importance to turbulent combustion [13, 23–25] and therefore merits further investigation for three-dimensional turbulent flow.

In summary, we have used the Kolmogorov-Petrovskii-Piskunov (KPP) equation with a random convection term, functional integral technique, and renormalization procedure to derive the crude upper bound for the ensemble-average speed of a reaction front in a turbulent shear flow in the limit of a large Reynolds number. We have found that the infrared divergence of turbulent flow may lead to the acceleration of the reaction front in the long-time, large-distance limit.

Note added. Since this paper was submitted the author has been informed by A. Majda that he and his co-workers have recently shown that due to intermittency, there is actually a much lower upper bound on the ensemble-averaged flame speed with a different scaling exponent (unpublished work).

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